LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040919\
Data File : BF113664.D
Acq On : 9 Apr 2019 16:34
Operator : JU/SJ
Sample : K2316-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190178-AMND-COMP-CS-5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.857	467	471	485	rBV	470888	644595	20.68%	2.154%
2	5.293	542	545	569	rBV	1790463	2126804	68.23%	7.106%
3	6.334	717	722	738	rBV	2742587	3032317	97.28%	10.132%
4	6.451	738	742	763	rVB	2871976	2697435	86.54%	9.013%
5	6.675	777	780	790	rBV	688279	668178	21.44%	2.233%
6	6.834	803	807	822	rVB	2518494	2240540	71.88%	7.486%
7	7.245	873	877	893	rBV	1941763	1931516	61.97%	6.454%
8	7.387	899	901	908	rVB	56702	60066	1.93%	0.201%
9	7.457	909	913	916	rVB	36730	33266	1.07%	0.111%
10	7.963	995	999	1017	rBV	808948	877390	28.15%	2.932%
11	8.498	1085	1090	1093	rBV	46328	40828	1.31%	0.136%
12	8.639	1110	1114	1118	rVB	316493	242551	7.78%	0.810%
13	8.728	1123	1129	1135	rBV	110470	174690	5.60%	0.584%
14	9.034	1177	1181	1189	rBV	3211258	2946090	94.51%	9.843%
15	9.098	1189	1192	1195	rVV	45747	43601	1.40%	0.146%
16	9.428	1245	1248	1253	rBV	435805	390585	12.53%	1.305%
17	9.663	1283	1288	1292	rBV	95586	147592	4.73%	0.493%
18	9.710	1292	1296	1308	rVB	1135684	1072500	34.41%	3.583%
19	10.498	1426	1430	1443	rBV	1600583	1643678	52.73%	5.492%
20	10.610	1445	1449	1452	rBV	272424	246600	7.91%	0.824%
21	10.792	1477	1480	1484	rVB	48047	41205	1.32%	0.138%
22	11.051	1521	1524	1529	rBV3	33730	57162	1.83%	0.191%
23	11.192	1544	1548	1556	rBV	1153078	1137528	36.49%	3.801%
24	11.363	1574	1577	1581	rBV3	36502	38720	1.24%	0.129%
25	11.727	1636	1639	1650	rBV3	288919	382160	12.26%	1.277%
26	12.404	1751	1754	1758	rBV	181242	170348	5.46%	0.569%
27	12.510	1769	1772	1778	rBV3	56689	74986	2.41%	0.251%
28	12.627	1787	1792	1798	rBV2	127043	190027	6.10%	0.635%
29	12.774	1812	1817	1820	rBV	3247624	3117078	100.00%	10.415%
30	13.069	1864	1867	1873	rVB4	23090	38470	1.23%	0.129%
31	13.345	1911	1914	1917	rBV	38766	36295	1.16%	0.121%
32	13.445	1928	1931	1935	rBV6	19515	31891	1.02%	0.107%
33	13.674	1967	1970	1976	rVB3	49832	55557	1.78%	0.186%
34	13.827	1988	1996	1999	rBV2	1026229	1338118	42.93%	4.471%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 20190178-AMND-COMP-CS-5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.986	2020	2023	2027	rVB	64654	58709	1.88%	0.196%
36	14.292	2072	2075	2078	rVB	98818	87416	2.80%	0.292%
37	14.586	2122	2125	2130	rVB	112551	104245	3.34%	0.348%
38	14.651	2132	2136	2140	rVB	140507	139032	4.46%	0.465%
39	14.839	2165	2168	2171	rBV	79346	101889	3.27%	0.340%
40	14.892	2174	2177	2183	rVB	127429	137736	4.42%	0.460%
41	15.115	2213	2215	2222	rVB	41652	51004	1.64%	0.170%
42	15.174	2222	2225	2230	rVB	49296	55141	1.77%	0.184%
43	15.233	2230	2235	2244	rBV	769607	978950	31.41%	3.271%
44	15.633	2299	2303	2308	rVB	63391	86994	2.79%	0.291%
45	16.086	2377	2380	2386	rVB2	37317	60169	1.93%	0.201%
46	16.610	2463	2469	2478	rVB3	41137	97867	3.14%	0.327%

Sum of corrected areas: 29929519

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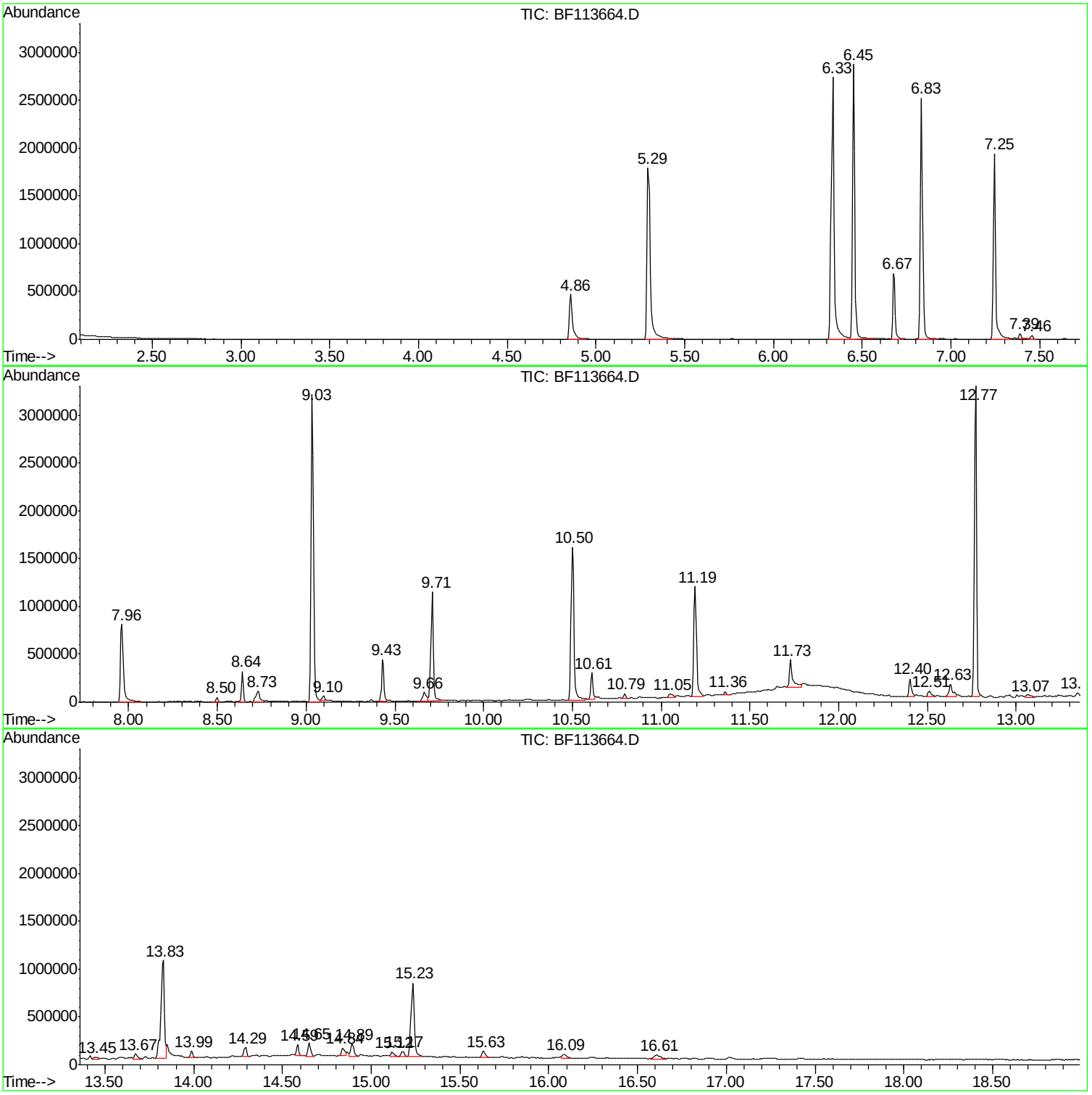
BNA_F
ClientSampleId :
20190178-AMND-COMP-CS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Data File : BF113664.D
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Operator : JU/SJ
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

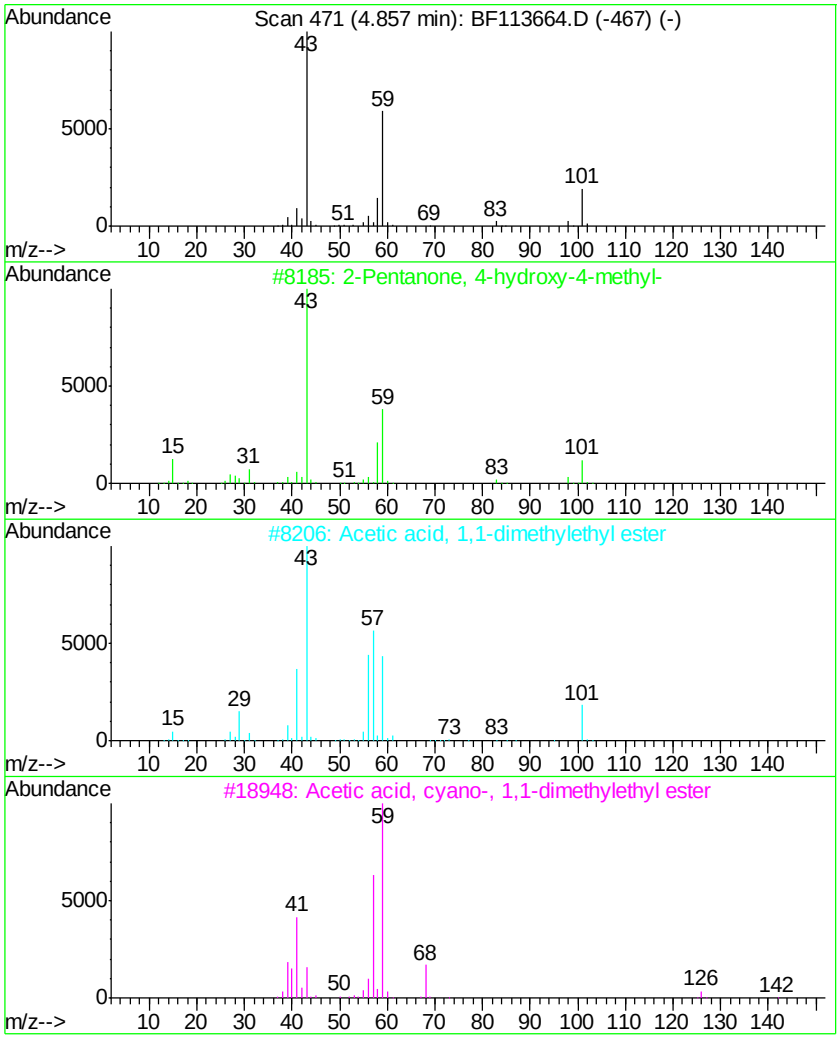
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

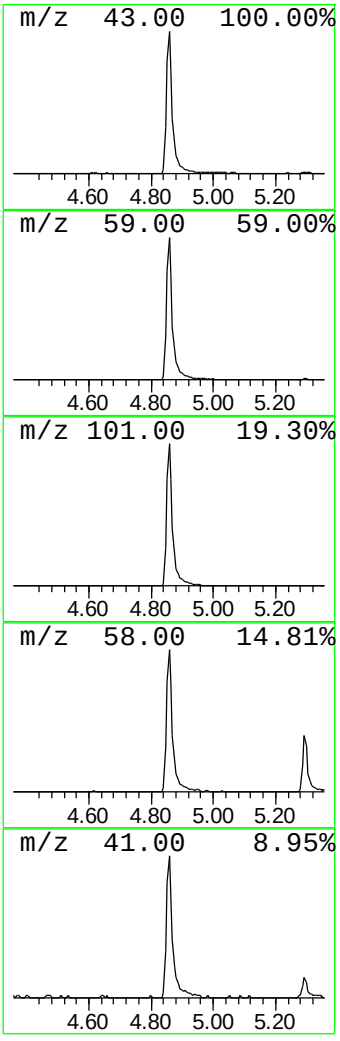
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	19.29 ng	644595	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_F
ClientSampleId : 20190178-AMND-COMP-CS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

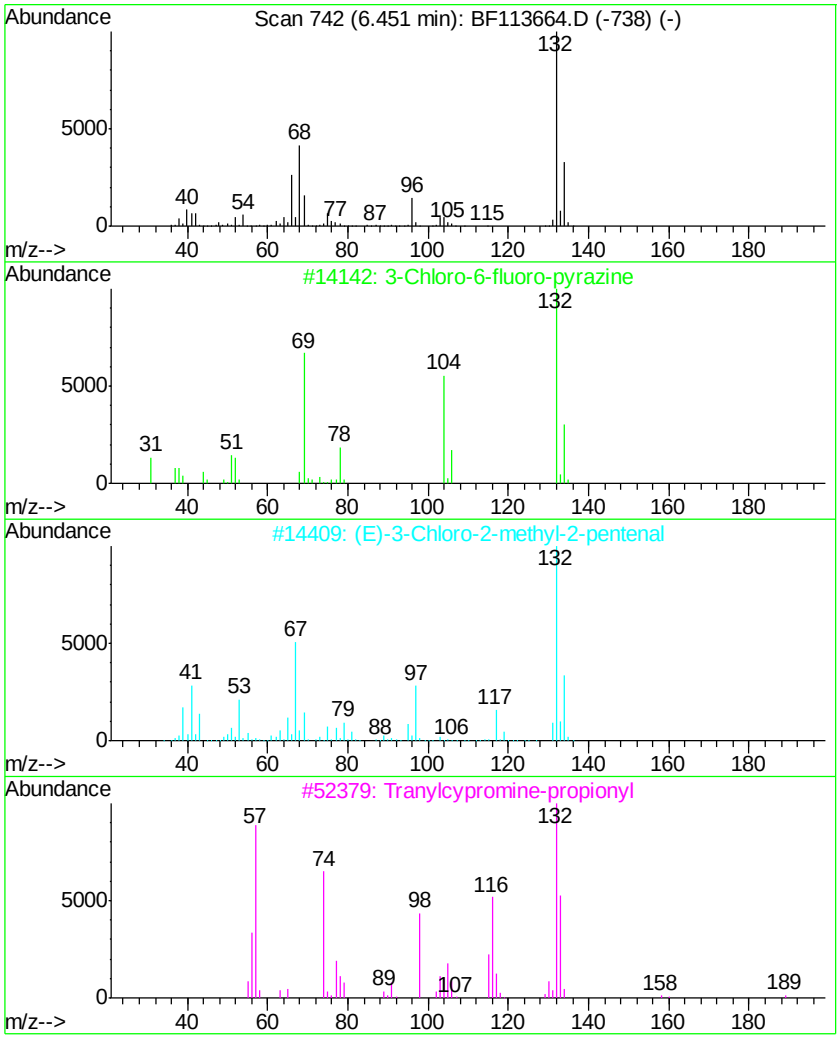
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

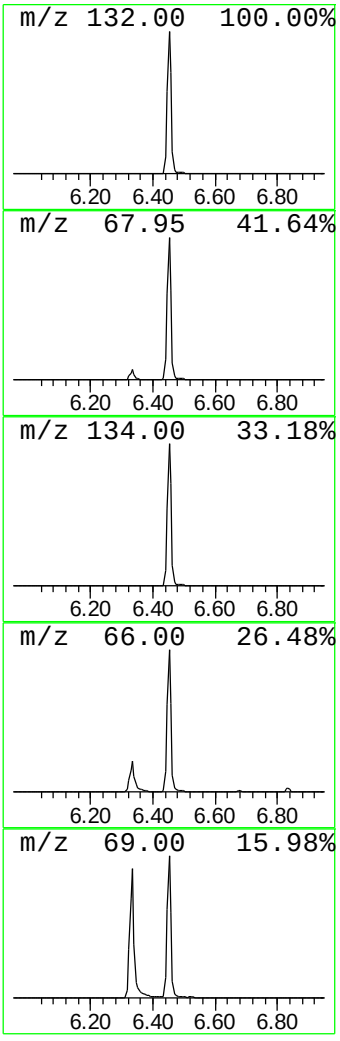
****

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	80.74 ng	2697440	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

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Sample : K2316-10
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20190178-AMND-COMP-CS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

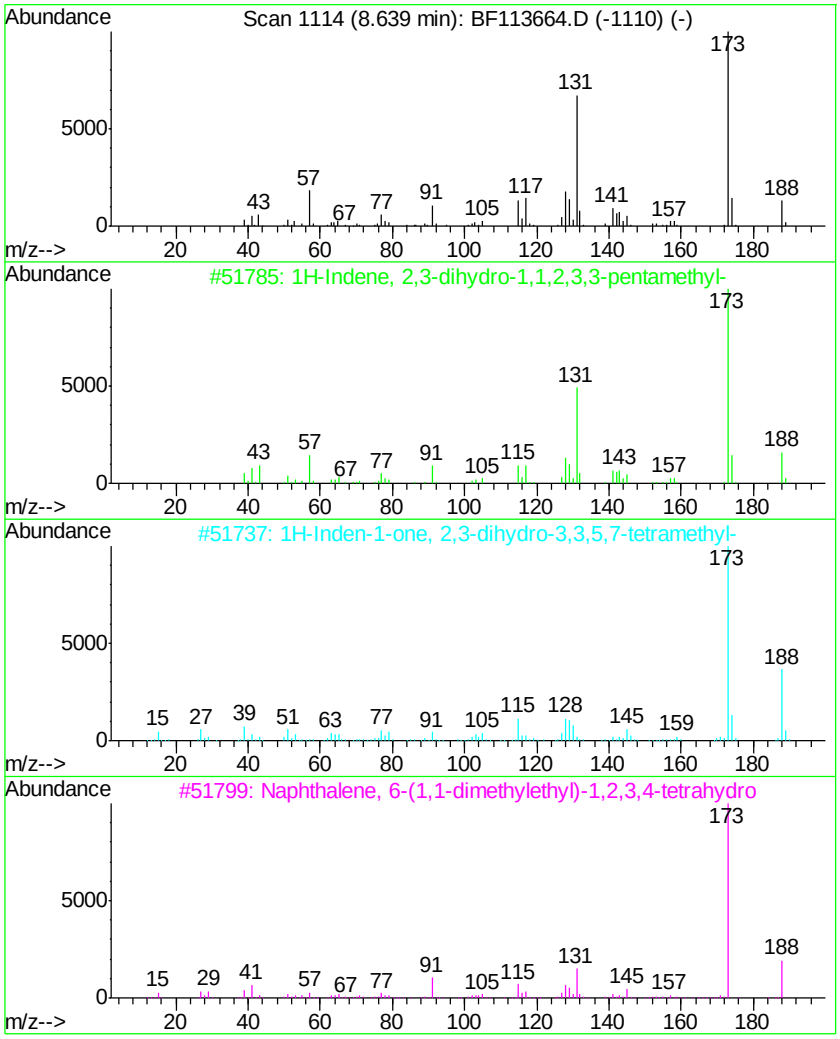
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

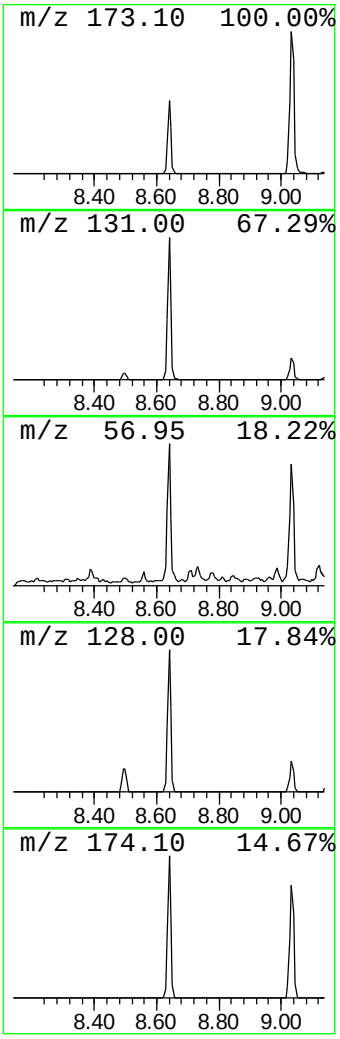
****

Peak Number 4 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.64	5.53 ng	242551	Naphthalene-d8	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,2,3,3...	188	C14H20	001203-17-4	97
2	1H-Inden-1-one, 2,3-dihydro-3,3,...	188	C13H16O	054789-23-0	49
3	Naphthalene, 6-(1,1-dimethylethy...	188	C14H20	042044-26-8	47
4	4H-1-Benzopyran, 4,4,5,8-tetrame...	188	C13H16O	082391-06-8	47
5	Benzimidazole, 5-tert-butyl-2-me...	188	C12H16N2	005805-62-9	43





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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190178-AMND-COMP-CS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

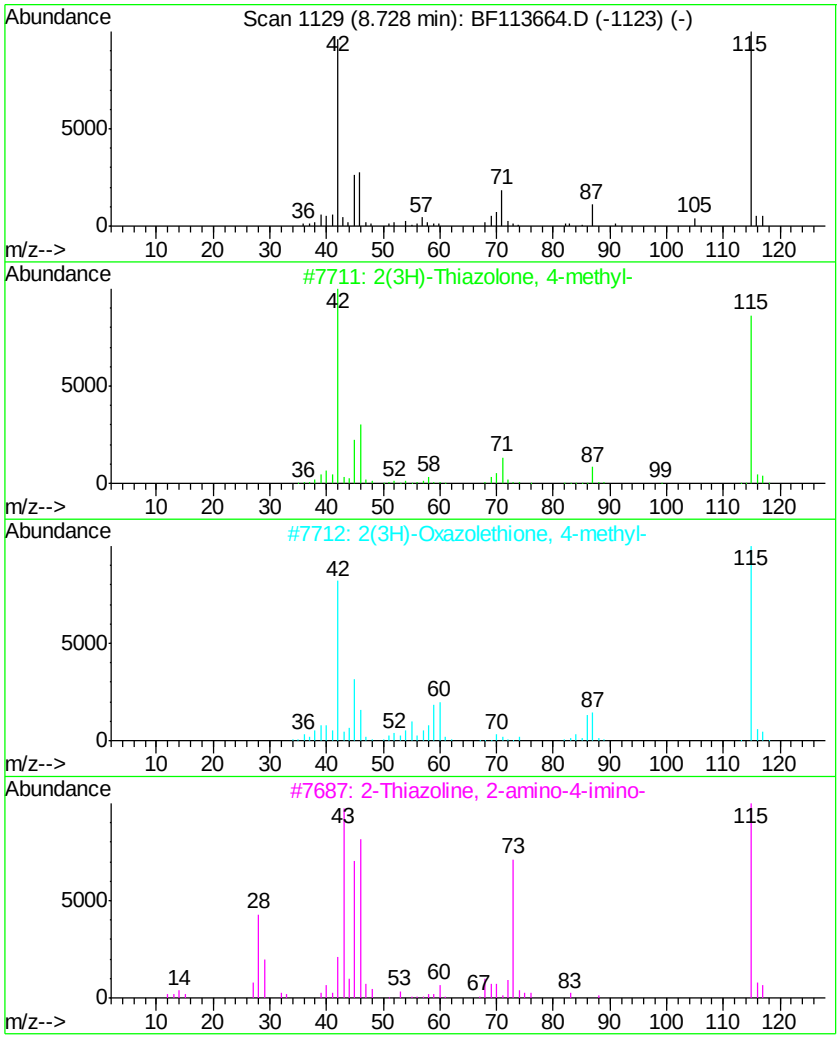
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

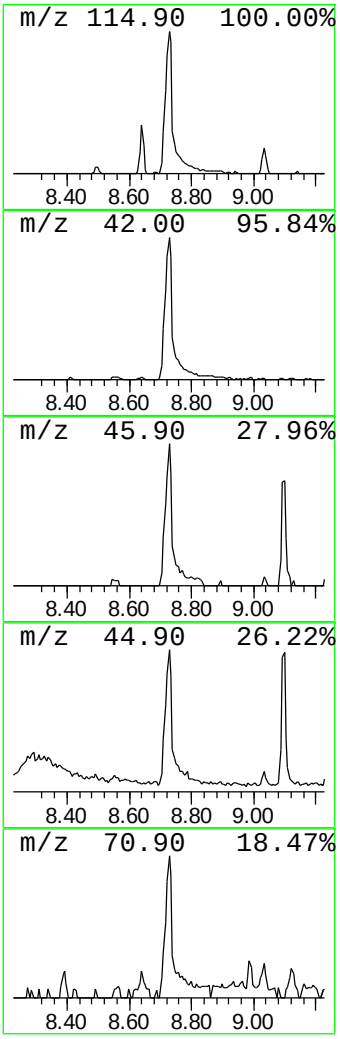
****

Peak Number 5 2(3H)-Thiazolone, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	3.98 ng	174690	Naphthalene-d8	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Thiazolone, 4-methyl-	115	C4H5NOS	032497-10-2	94
2	2(3H)-Oxazolethione, 4-methyl-	115	C4H5NOS	013016-17-6	86
3	2-Thiazoline, 2-amino-4-imino-	115	C3H5N3S	026246-29-7	37
4	Thiazole, 5-methoxy-	115	C4H5NOS	014542-14-4	16
5	1H-1,2,4-Triazole, 3-thiol-5-met...	115	C3H5N3S	007271-44-5	12





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TIC Library : C:\DATABASE\NIST11.L
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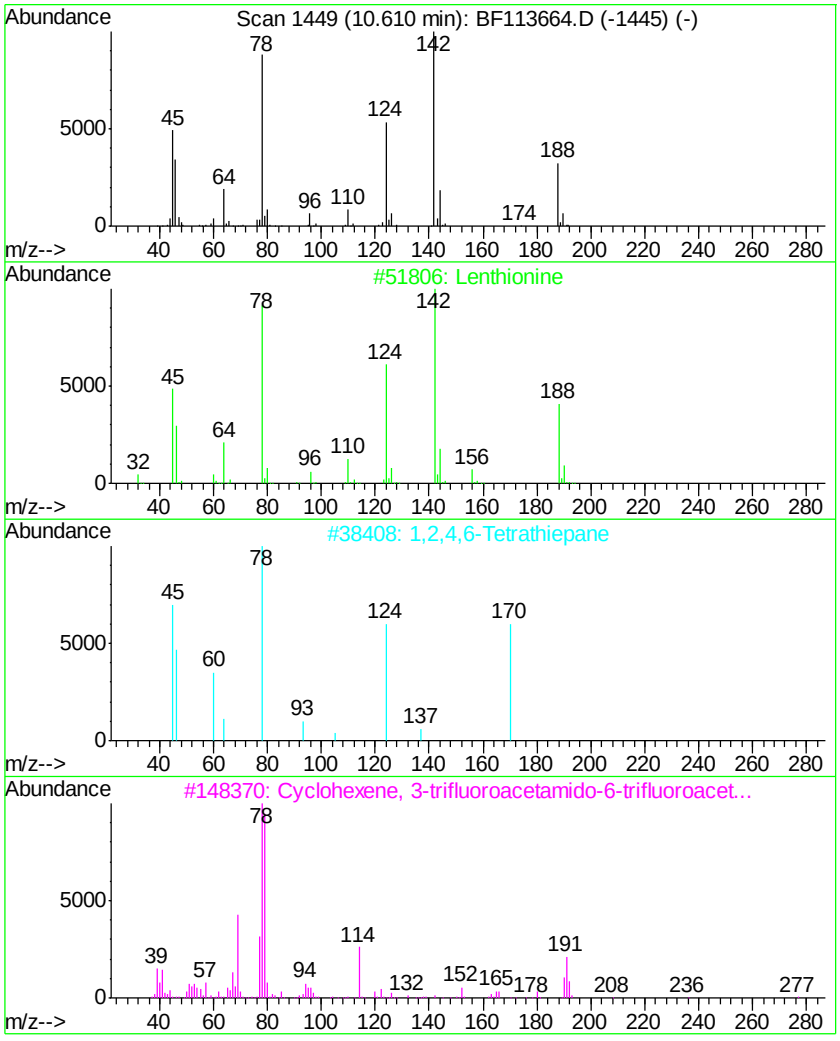
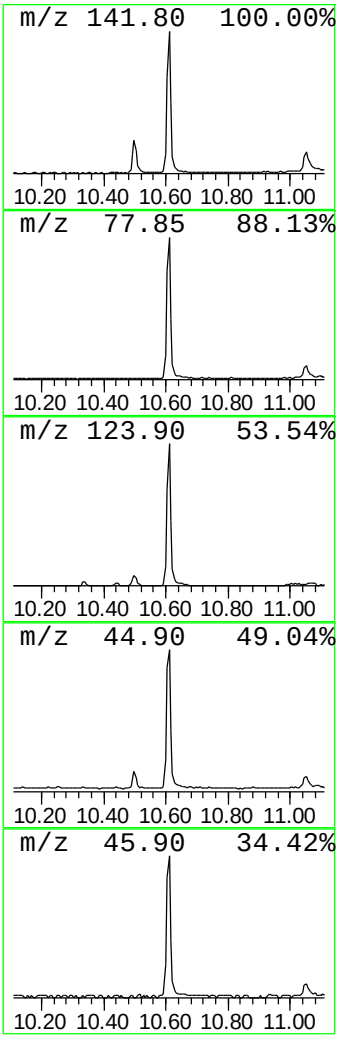
****

Peak Number 6 Lenthionine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	4.34 ng	246600	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	98
2	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	38
3	Cyclohexene, 3-trifluoroacetamid...	305	C10H9F6NO3	1000153-70-3	25
4	1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9
5	Boronic acid, phenyl-	122	C6H7BO2	000098-80-6	9





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Instrument : BNA_F
ClientSampleId : 20190178-AMND-COMP-CS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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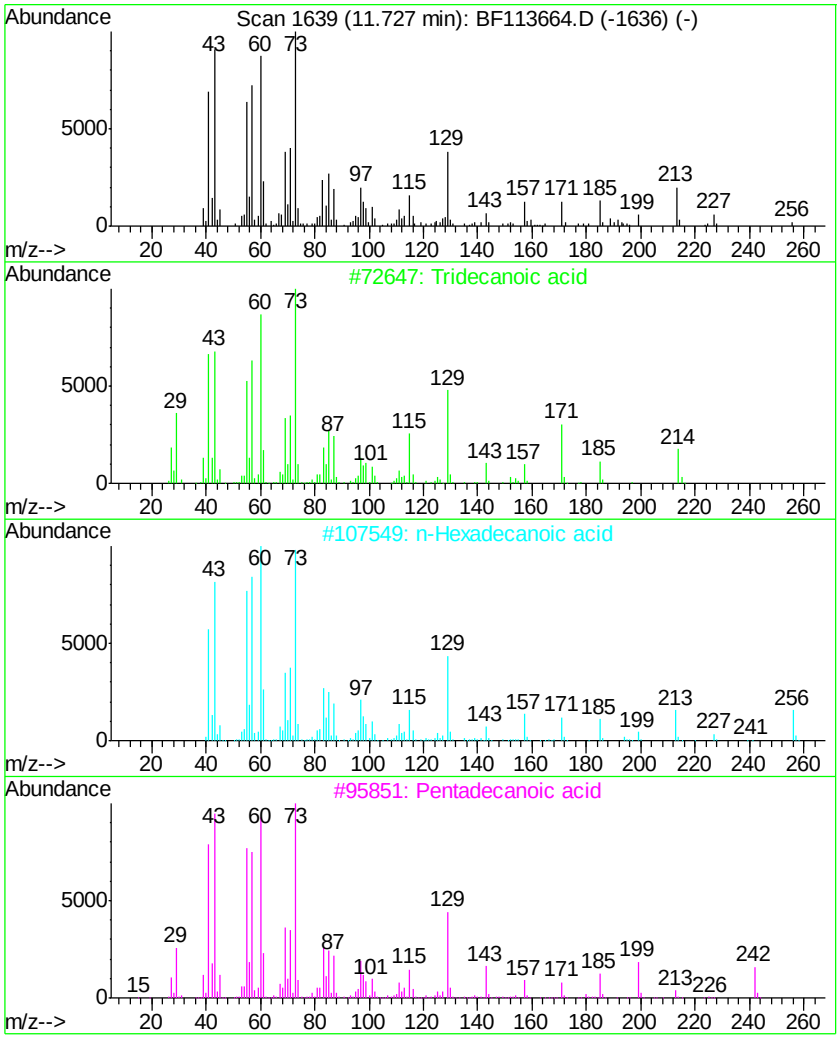
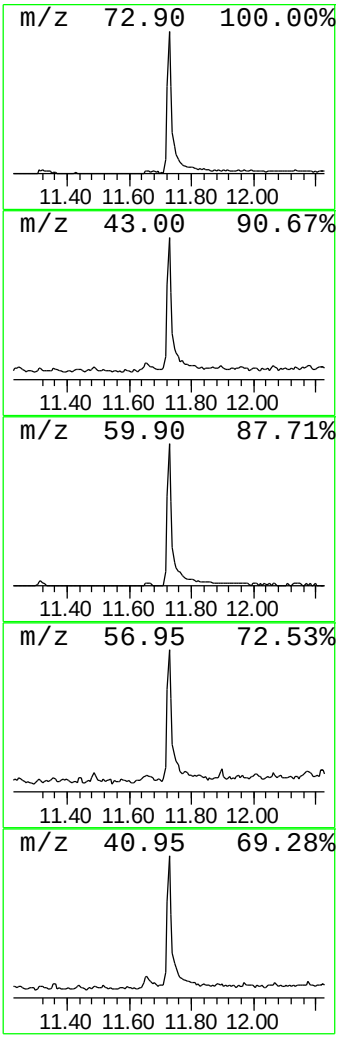
Peak Number 7 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	6.72 ng	382160	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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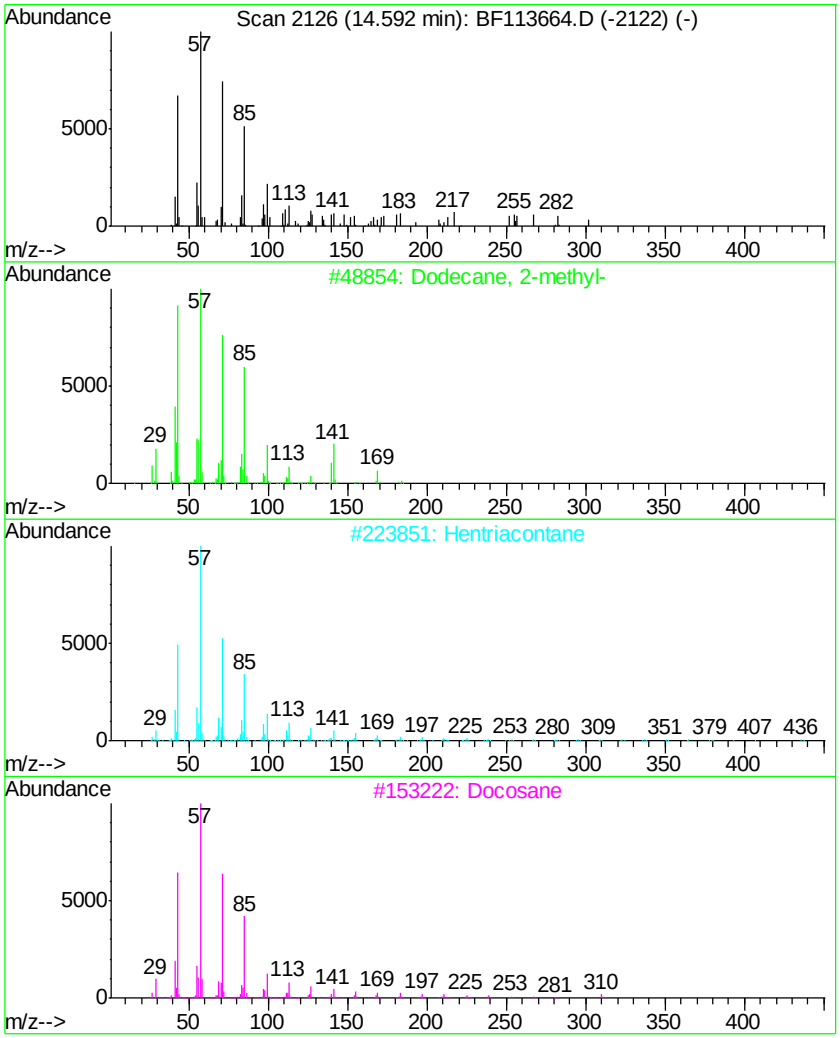
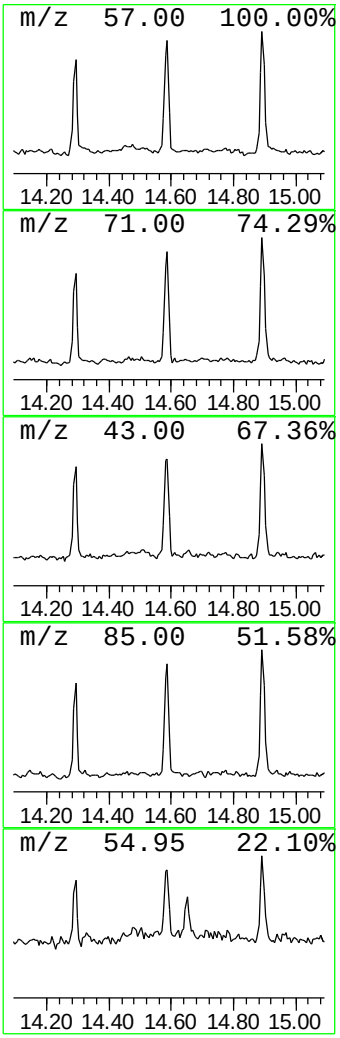
Peak Number 8 Dodecane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.13 ng	104245	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Docosane	310	C22H46	000629-97-0	86
4	Heneicosane	296	C21H44	000629-94-7	86
5	Tridecane, 3-methyl-	198	C14H30	006418-41-3	86





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Data File : BF113664.D
Acq On : 9 Apr 2019 16:34
Operator : JU/SJ
Sample : K2316-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190178-AMND-COMP-CS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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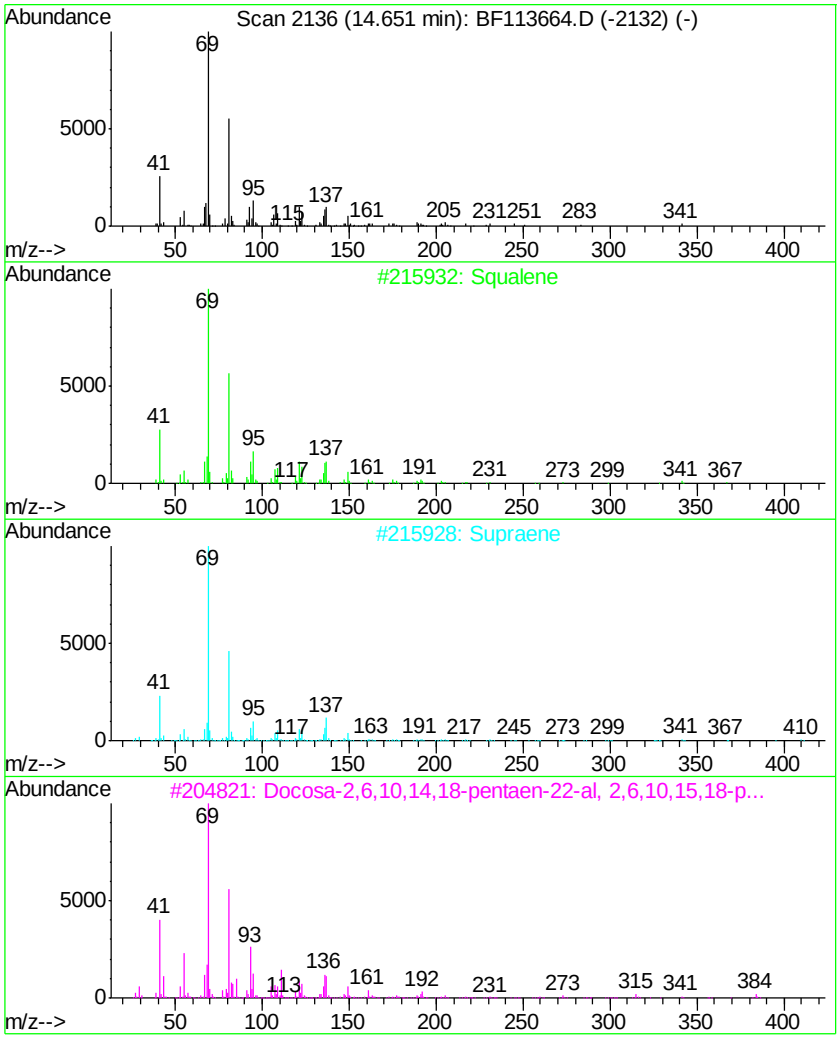
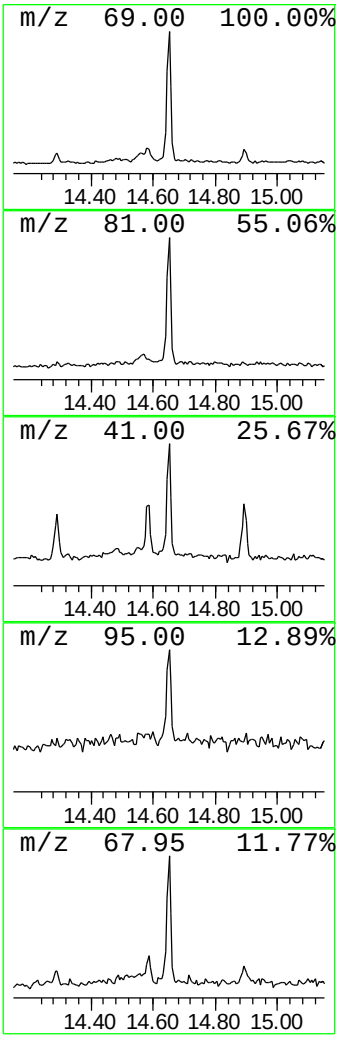
Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.84 ng	139032	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040919\
Data File : BF113664.D
Acq On : 9 Apr 2019 16:34
Operator : JU/SJ
Sample : K2316-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20190178-AMND-COMP-CS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

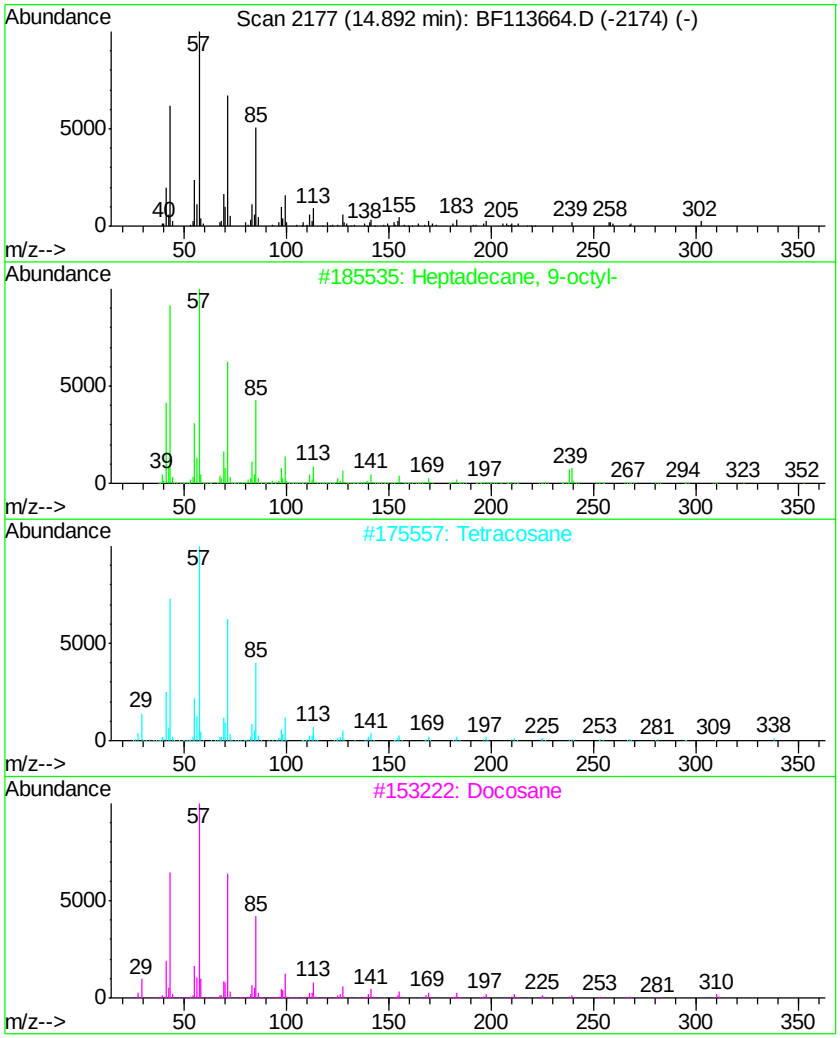
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

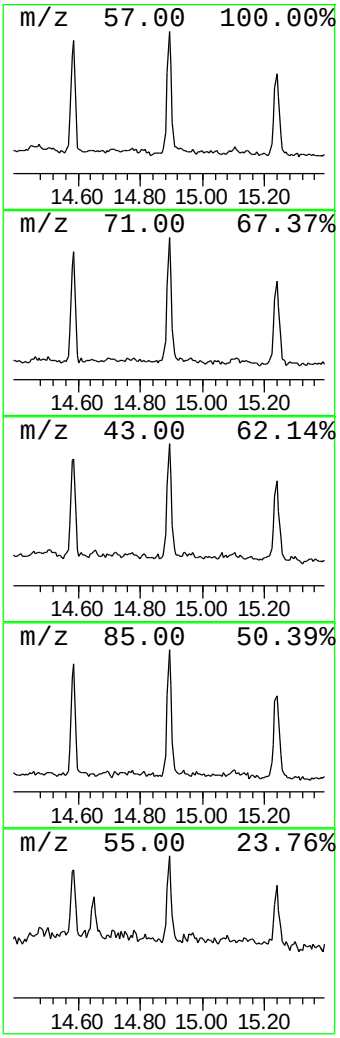
****

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.81 ng	137736	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
2	Tetracosane	338	C24H50	000646-31-1	87
3	Docosane	310	C22H46	000629-97-0	87
4	Hexacosane	366	C26H54	000630-01-3	86
5	Heneicosane	296	C21H44	000629-94-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040919\
Data File : BF113664.D
Acq On : 9 Apr 2019 16:34
Operator : JU/SJ
Sample : K2316-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190178-AMND-COMP-CS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.86	19.3	ng	644595	1	6.67	668178	20.0
unknown6.45	6.45	80.7	ng	2697440	1	6.67	668178	20.0
1H-Indene, 2,3-di...	8.64	5.5	ng	242551	2	7.96	877390	20.0
2(3H)-Thiazolone,...	8.73	4.0	ng	174690	2	7.96	877390	20.0
Lenthionine	10.61	4.3	ng	246600	4	11.19	1137530	20.0
Tridecanoic acid	11.73	6.7	ng	382160	4	11.19	1137530	20.0
Dodecane, 2-methyl-	14.59	2.1	ng	104245	6	15.23	978950	20.0
Squalene	14.65	2.8	ng	139032	6	15.23	978950	20.0
Heptadecane, 9-oc...	14.89	2.8	ng	137736	6	15.23	978950	20.0